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SUMMARY OF THE FOURTH MEETING OF THE SCIENTIFIC ADVISORY BOARD'S TEMPORARY WORKING GROUP ON CHEMICAL FORENSICS 22 – 24 JANUARY 2025

1. AGENDA ITEM ONE – Opening of the meeting and adoption of the agenda

1.1 The Temporary Working Group (TWG) on Chemical Forensics of the Scientific Advisory Board (SAB) held its fourth meeting from 22 to 24 January 2025. The meeting was chaired by Dr Anne Bossée on behalf of the SAB, with Dr Simon Ovenden as Vice-Chairperson.

1.2 Dr Bossée opened the fourth meeting of the TWG by warmly welcoming its members and the external speakers and inviting all participants to introduce themselves. A list of participants appears in the Annex to this report. She acknowledged the valuable contributions that the presentations of the external speakers bring to the TWG's findings. Dr Bossée recalled that, with Dr Ovenden, she had compiled a first draft of the end-of-mandate report, which had been circulated to subgroup leads in December 2024. This text had been discussed in each subgroup and would continue to be discussed throughout this fourth meeting. She underscored the importance of reviewing the text and identifying any outstanding gaps so that external speakers on specific topics may be sought for the next meeting of the TWG.

1.3 As no objections or comments were raised in response to the proposed programme of work during the three days of the meeting, the following agenda was adopted:

1. Opening of the meeting and adoption of the agenda
2. Updates from subgroups[1]
3. Beyond Industry and Traffic: Unveiling the Hidden Sources of Urban Air Pollution
4. New resources for chemical forensics
5. Metabolomics at Repository Scales: Leveraging Mass Spectrometry Big Data to Illuminate Dark Matter
6. National Measurement Institute – Australian Forensic Drug Laboratory's Profiling Program

[1] While agenda items 2, 9, 12, and 13 were discussed separately during the meeting, they are reported herein under a single agenda item for clarity and to minimise duplication.

7. A Police Perspective on Chemical Forensics and Chemometrics: ENFSI Projects STEFA and ROTOR

8. Evidence-based assurance and verification of Australian agriculture provenance

9. Subgroups breakout sessions[2]

10. Casework examples of fire debris analysis and miscellaneous chemical investigations in the Netherlands

11. Challenges for chemical forensics and chlorine profiling in concrete

12. Subgroups breakout sessions[3]

13. Group discussion[4]

14. Closing remarks and any other business

15. Closure of the meeting

2. AGENDA ITEMS TWO, NINE, TWELVE, AND THIRTEEN – Discussions on subgroup topics

2.1 Subgroup 1, led by Dr Crister Åstot, is focusing on the state of the art of chemical forensics, and is considering the areas of batch matching, impurity profiling, synthesis routes, geographical and environmental factors, and isotope ratios. It was highlighted that both profiling, which is knowing about the synthetic pathways and routes, and batch matching support efforts to prevent the re-emergence of chemical weapons.

2.2 During the intersessional period as well as the fourth TWG meeting, Subgroup 1 continued formulating and refining recommendations to improve the availability of reference data and to maintain and further enhance chemical forensics capabilities at the OPCW, ensuring that these recommendations are implementable and effective. The subgroup agreed that integrating the expertise of statisticians and data scientists within the Technical Secretariat (the Secretariat) could support these efforts. The subgroup also discussed the importance of ensuring and enhancing national capacities in sampling and subsequent analysis. Generally, as much information as possible should be collected from a sample for potential (future) forensic investigations, which may include spectra from detection and identification devices in the field.

2.3 The subgroup underscored the importance of ensuring that the Secretariat maintain and further enhance its chemical forensics capabilities for future missions, noting the important chemical forensics-related work for the Syrian Arab Republic being conducted by the non-routine missions and ensuring that the knowledge and expertise gained is sustained moving forward.

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2 Ibid.

3 Ibid.

4 Ibid.

2.4 Reference data were discussed extensively. Subgroup 1 noted the lack of ground truth reference data relating to chemical warfare agents compared to the criminal sciences, and how this limits the statistical strength of the applied methods. The subgroup discussed leveraging artificial intelligence (AI) to predict additional reference data, through data augmentation, for example, but agreed that more empirical results would be more beneficial. Subgroup 1 also discussed the required size of a reference database to support the application of a likelihood ratio-based approach to inform expert opinions in investigations, including those involving chemical weapons. Invited speakers Mr Sami Huhtala and Dr Michiel Grutters, from the forensic laboratories of Finland and the Netherlands, respectively, emphasised the compelling value of this statistical approach in forensic investigations. However, they also highlighted the ongoing need for sufficient and relevant reference data.

2.5 Subgroup 1 also discussed information sharing. The subgroup members noted the reluctance of States Parties to share existing data through concern that this may reveal sensitive production information. The group further noted that, regarding chemical forensics work, two-way communication between designated laboratories and operational units, such as the non-routine missions, may augment the investigations as the laboratory analysis may benefit from additional information about the samples in question, particularly in an iterative process throughout the analysis.

2.6 Dr Grégoire Delaporte, Subgroup 2 lead, reported that, during the intersessional period, the literature review on the application of AI/machine learning (ML) methods in the broader fields of chemistry and forensic science was completed. Based on the findings, an inventory of ML methods used in chemical forensics had been compiled and further developed. This will form an important output of Subgroup 2. A glossary of key AI/ML terms has also been developed.

2.7 During the fourth meeting of the TWG, the objectives of Subgroup 2 were to further discuss and agree the structure of its contribution to the end-of-mandate report and to review the proposed content to identify any potential gaps. The subgroup members highlighted that the rapid developments in ML will have a growing influence on the field of chemical forensics and there is a need to make sure the chemical weapons analysis community benefits from these developments. They discussed the benefits of using large language models to stay apprised of relevant developments, which can be helpful in quick-moving areas like analytical chemistry, and the fact that these models may also be able to detect non-intuitive inferences and hard-to-perceive connections. The subgroup also discussed how to identify tools and techniques from other fields, including analytical chemistry, omics sciences, and environmental monitoring, that may be directly applicable to chemical forensics, and advocated for both intra- and inter-field collaboration.

2.8 Subgroup 2 also considered further the existing obstacles for designated laboratories in implementing ML methods for chemical forensic purposes. These include the need for staff with information technology skills, inability to access tools using web services due to sensitivity concerns, availability of tools suitable for small-scale or limited data sets, and the ability to share data between laboratories. With these obstacles in mind, Subgroup 2 will continue to refine its potential recommendations during the intersessional period.

2.9 Ms Ang Lee Hwi, Subgroup 3 lead, provided updates on the work undertaken during the intersessional period. She noted that regarding the task of reviewing relevant published standards and best practices for forensic science, including International Organization for Standardization/International Electrotechnical Commission (ISO/IEC) standards, the subgroup had compiled and gathered a list of the relevant documents. Based on a preliminary review, laboratories performing forensic analyses of chemical weapons and chemical weapons-related substances should already have a robust quality management system in place. Ideally, testing laboratories should already be meeting, or taking steps towards meeting, ISO/IEC Standard 17025 requirements (or those of the International Forensic Strategic Alliance), with specific requirements for forensic laboratories (relevant to their accreditation bodies). Ms Ang reported that Subgroup 3 is continuing to review the guidelines and refine its potential recommendations for the final report.

2.10 Subgroup 3 continued its discussions regarding the review of published standards and best practices during the fourth meeting of the TWG. It shortlisted documents which will enable it to gather information on the specific requirements for on-site sampling and chemometrics method and validation. The subgroup will review the documents in the upcoming intersessional period and update specific recommendations at the next TWG meeting.

2.11 During the fourth meeting of the TWG, the subgroup further discussed the need to better understand how combining analysis techniques, and data therefrom, can yield additional important information. The purpose of chemical forensics is to provide information beyond verification and generate leads for the investigation (for example, how a compound has been made, where it was made, etc.). The data from various techniques could provide different leads that could be leveraged together to aid the investigation, using an approach to combine results rather than combine data. Subgroup 3 proposed that it may be more appropriate and effective to engage laboratories with complementary expertise for the analysis of the same set of samples, rather than using the current verification practice where laboratories with the same expertise are engaged to confirm the identification. It was also suggested that a framework for combining results could be established through confidence-building exercises.

2.12 With respect to its discussions on developing a database, Subgroup 3 considered privacy-preserved data sharing, a critical prerequisite for database building. The current system that the OPCW adopts for the submission of declaration data could be a positive demonstration of such a secure system. Dr Nina Welti, an invited speaker with experience in this area, shared information on different privacy preservation methods, including the addition of synthetic data to real-world data. During the next intersessional period, the subgroup will further consider the types of data (for example, raw data, lists of chemical attribution signatures, etc.) to collect for the database. Subgroup 3 also noted that different types of forensic databases may be possible. These could include expanding the OPCW Central Analytical Database (OCAD) by adding relevant data on a specific synthesis pathway or creating an entirely new forensic database based on the profiles of Schedule 1 chemicals in raw samples. As these different types of database structures would not have the same degree of data sensitivity, this approach may overcome existing reluctance to voluntarily share data. The possible types of forensic databases, with their associated pros and cons, will be discussed at the fifth meeting of the TWG.

2.13 During the intersessional period, Subgroup 4—led by Dr Hanna Hakulinen—continued to explore potential scenarios of chemical warfare agent use and related chemical forensics methodologies, to help identify key questions and gaps in investigations. Dr Hakulinen stated that she has been developing the contribution of Subgroup 4 to the end-of-mandate report, and noted that the table of capabilities requires further group discussion, noting that overlaps with other subgroup inputs will be deconflicted.

2.14 During the fourth meeting, a number of topics relating to the subgroup's work were discussed. This included the roster of non-designated laboratories, specifically which laboratories to include and how the roster should be developed, and the content for inclusion in the capabilities matrix. In the context of sampling, consideration was given to situational awareness and the need to harmonise sampling, as well as any first response activities, and an example of regional collaboration was highlighted. The development and content of the proposed database were also the focus of discussions. Subgroup 4 proposed that the database could complement the OCAD (data on scheduled chemicals used for verification purposes) by providing data on scheduled and non-scheduled chemicals, such as route-specific impurities, together with the related metadata and references to published literature. The members noted the importance of the Validation Group in this process, and that validation requirements will need to be carefully defined and communicated. Furthermore, the validation of verification data will have requirements different to those for the validation of chemical forensics data.

2.15 Subgroup 4 considered confidence-building exercises in detail and proposed that existing methods (such as the recommended operating procedures in the VERIFIN Blue Book) should be tested and updated when necessary. Working in teams will be tested in the upcoming Chemical Forensics International Technical Working Group (CFITWG) Icarus exercise. Additional discussions focused on how existing designated laboratories with chemical forensics capabilities could be determined, and on how the dissemination to these laboratories in the coming months of a questionnaire on existing capabilities would benefit the development of the capabilities matrix. Reporting forensics results was discussed at length and the subgroup agreed to follow up on this topic during the next intersessional period.

2.16 Finally, Subgroup 4 carefully reviewed all its proposed recommendations and agreed to continue to think about these moving forward.

3. AGENDA ITEM THREE – Beyond Industry and Traffic: Unveiling the Hidden Sources of Urban Air Pollution

3.1 Dr Georgios Gkatzelis, from the Forschungszentrum Jülich GmbH, Germany, described the work of his research group to better understand the causes behind, and constitution of, air pollution. Air pollution is one of the largest human health risk factors globally, causing 6.7 million premature deaths per year. Over half of the world's population currently lives in urban areas, and this number is expected to continue growing. The most relevant pollutant for health impacts included in the World Health Organization guidelines is fine particulate matter with a diameter smaller than 2.5 μm, also called PM2.5. A significant fraction of the PM2.5 mass consists of organic aerosols composed of hundreds to thousands of compounds. Primary organic aerosols are

directly emitted into the atmosphere, from sources such as vehicles, cooking,[5] and the burning of biomass. Contrarily, secondary organic aerosols (SOAs) are formed via diverse chemical reactions that transform more volatile precursors, such as volatile organic compounds (VOCs), into lower-volatility products that either condense into existing particles or form new particles. Studies have shown that a significant fraction of urban particulate matter pollution is from anthropogenic SOAs, however many of the developed chemical transport models underpredict the amount of urban SOAs, as compared to experimentally measured amounts, with high variability. Current studies indicate that existing anthropogenic SOA models miss some level of contribution from a gas-phase source.

3.2 Historically, combustion sources and motor vehicles have been responsible for most VOC emissions measured in outdoor urban environments that can act as precursors for anthropogenic SOA formation. In recent work, Dr Gkatzelis has shown that volatile chemical products (VCPs) from household chemicals,[6] such as personal care products, cleaning agents, coatings, pesticides, printing inks, and adhesives, have emerged as the largest source of petrochemical VOC emissions relative to combustion sources in densely populated cities in the United States of America and Europe.[7] In a pilot study performed in New York City, Dr Gkatzelis and his team concluded that VCPs account for over half of the anthropogenic VOC emissions.[8] However, the impacts of VCPs on anthropogenic SOA formation are not understood. Although recent model studies promote that this emission source could bridge the gap between observed and modelled anthropogenic SOAs, to date there are no ambient measurements to support this.

3.3 The combination of an anticipated decrease in combustion-related emissions due to ongoing global defossilisation efforts and the continued increase in the global population density of cities indicates that VCP emissions are expected to dominate the urban air. This is supported by recent research that showed that even with a considerable decrease in the emission of urban nitrogen oxides due to COVID-19 lockdown measures, PM2.5 concentrations did not drastically decrease. Given the current knowledge gap in predicting anthropogenic SOA and the observed PM2.5 levels even during lockdowns, it is essential to identify the precursors of urban secondary pollution to advise future adaptation policies to improve air quality and reduce health impacts in urban air.

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5 Coggon, M. M., C. E. Stockwell, L. Xu, J. Peischl, J. B. Gilman, A. Lamplugh, H. J. Bowman, et al. "Contribution of Cooking Emissions to the Urban Volatile Organic Compounds in Las Vegas, NV." *Atmospheric Chemistry and Physics* 24, no. 7 (April 12, 2024): 4289–4304. https://doi.org/10.5194/acp-24-4289-2024.

6 McDonald, B. C., J. A. de Gouw, J. B. Gilman, S. H. Jathar, A. Akherati, C. D. Cappa, J. L. Jimenez, et al. "Volatile Chemical Products Emerging as Largest Petrochemical Source of Urban Organic Emissions." *Science* 359, no. 6377 (February 16, 2018): 760–64. https://doi.org/10.1126/science.aaq0524.

7 Gkatzelis, G. I., M. M. Coggon, B. C. McDonald, J. Peischl, K. C. Aikin, J. B. Gilman, M. Trainer, and C. Warneke. "Identifying Volatile Chemical Product Tracer Compounds in U.S. Cities." *Environmental Science & Technology* 55, no. 1 (December 16, 2020): 188–99. https://doi.org/10.1021/acs.est.0c05467.

8 Coggon, M. M., G. I. Gkatzelis, B. C. McDonald, J. B. Gilman, R. H. Schwantes, N. Abuhassan, K. C. Aikin, et al. "Volatile Chemical Product Emissions Enhance Ozone and Modulate Urban Chemistry." *Proceedings of the National Academy of Sciences* 118, no. 32 (August 2, 2021). https://doi.org/10.1073/pnas.2026653118.

3.4 The Gkatzelis research group aims to address this major scientific gap by performing field observations and controlled simulation chamber experiments with various state-of-the-art mass spectrometry (MS) instruments deployed in different ways, including:

(a) in a mobile laboratory for measurements at emission hot spots where urban emissions from traffic, cooking, and VCPs are the dominant pollution sources;

(b) for ground-based, longer-term observations on the timescale of one to two months to quantify the contribution of multiple urban sources as well as the influence of biogenic emissions;

(c) in a specialised atmosphere simulation chamber, SAPHIR, for controlled atmospherically relevant oxidation of multi-precursor VCP mixtures, traffic-related mixtures, and their combination, to form anthropogenic SOAs; and

(d) on a Zeppelin airship for targeted flights to capture the urban enhancement and evolution of gas-phase pollutants to produce anthropogenic SOAs over cities.

3.5 Following his presentation, TWG members discussed several elements of the presentation by Dr Gkatzelis. These included the limitations when performing MS in an airborne setting, the various types of biogenic pollution, the effects of ozone in the stratosphere compared to the troposphere, and the possibility of using the SAPHIR (Simulation of Atmospheric Photochemistry in a Large Reaction Chamber) experiment for scenarios involving scheduled chemicals. Dr Gkatzelis further explained that cars introduce pollutants such as nitrogen oxides into the atmosphere and they contribute to the creation of ozone in populated areas.

4. AGENDA ITEM FOUR – New resources for chemical forensics

4.1 Prof. David Wishart, from the University of Alberta, Canada, gave an overview of recent advances in his laboratory in the area of chemical forensics, particularly in the context of identifying, quantifying, and understanding chemical compounds for forensic chemistry applications. He began by highlighting some of the challenges faced in the chemical forensics space before highlighting four specific areas that would benefit from better methods: identifying and understanding known compounds; identifying and quantifying known compounds in more standardised ways; predicting biotic and abiotic transformations; and identifying unknown as well as "unknown unknown" compounds. Prof. Wishart stressed that the overarching goal is to enhance the accuracy and reliability of chemical analyses to address issues ranging from environmental monitoring to criminal investigations. The remainder of his presentation was divided into four parts.

4.2 Prof. Wishart focused first on the topic of identifying and understanding known compounds. Current existing spectral and chromatographic databases have limitations, including the lack of detailed compound annotations and the lack of support for multispectral searching or multispectral integration. To overcome these limitations, his research group had developed several resources that provide detailed compound annotation and offer support for multispectral searching. These include the Human Metabolome Database (HMDB), DrugBank, the Toxic Exposome Database (T3DB), and ContaminantDB, which provide rich annotations, predicted spectra, and

user-friendly interfaces.[9] These resources are designed to be FAIR-compliant (findable, accessible, interoperable, reusable) and aim to democratise access to chemical forensic tools globally.

4.3 Prof. Wishart then detailed his team's use of AI and ML for predicting spectral and chemical properties, filling gaps in experimental data, and supporting the identification of both known and unknown compounds. Tools like CFM-ID, FraGNNet, PROSPRE, Caspre, and RT Pred have been used for accurately predicting retention times and spectral data, and for facilitating the identification of known compounds through multispectral search methods.

4.4 The discussion then turned to approaches to identifying and quantifying known compounds in more standardised ways. Omics, such as metabolomics or exposomics, either targeted or untargeted, can be useful in chemical forensics applications. Prof. Wishart's group has developed targeted, standardised kits and ISO standardised assays for quantitatively measuring a wide variety of compounds using metabolomics and exposomics principles. These include kits for nuclear magnetic resonance (NMR) spectroscopy, gas chromatography-mass spectrometry (GC-MS), and liquid chromatography-mass spectrometry (LC-MS). The "kitification" of targeted assays allows for up to 1,800 compounds to be quantitatively measured in just a few minutes for a few dollars per sample. Low-cost robotic systems have been developed to make the process even simpler and more robust. This automation allows users to implement a "load and leave" operation, which further reduces cost and further enhances reproducibility. These kits have been adapted for many applications (for example, exposomics, food/beverage testing, and drug testing) and have been used by various research groups around the world.

4.5 Prof. Wishart then shifted focus to discuss predicting biotic and abiotic transformations. Many compounds, when detected, are not found in their original, pure state, but have gone through significant chemical or biological transformations due to ingestion or environmental degradation. This makes their identification or the identification of the source material more difficult. And while most compounds that are manufactured by humans or synthesised by plants and animals are already known, their biotic and abiotic transformation products are mostly unknown. These unknowns are called the "dark matter". Current estimates size the "dark matter" at about 25 million compounds, around 50 times the number of known, high-abundance compounds. BioTransformer was developed to predict both biotic and abiotic transformation reactions, generating not only novel structures, but also providing multi-step reaction process information.[10] Prof. Wishart's group is currently running all known compounds in its databases through BioTransformer to generate a database called TransformDB, which contains millions of novel structures along with information about the reactions that led to them. Spectral prediction tools are then being used to generate predicted NMR, MS, tandem mass spectrometry (MS/MS), retention time, and retention index data for all these novel compounds. When complete, users will be able to identify many previously unknown compounds (that is, the dark matter) and trace their possible origins, in a few seconds, simply with a click of a button.

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9 For more information, see: https://hmdb.ca (HMDB); https://go.drugbank.com/ (DrugBank); and https://t3db.ca (T3DB). ContaminantDB will be formally released in 2025.

10 For more information, see: https://biotransformer.ca.

4.6 Lastly, Prof. Wishart discussed the challenge of identifying unknown compounds and "unknown unknown" compounds. Current approaches to the identification of unknowns tend to focus on spectrum-to-compound methods, but these have limitations. A compound-to-spectrum method may also be used to predict likely "unknown" compounds based on predicted spectra of known compounds, via tools like BioTransformer. He then discussed the concept of generative modelling and how chemical language models can serve as an alternative route to generating novel, but chemically or biologically feasible, structures. Chemical language models have been used to create millions of structures of predicted novel psychoactive substances, predicted human metabolites, and predicted plant or food compounds, many of which were later found to exist or were detected in subsequent studies. Prof. Wishart gave an overview of tools and webservers like DarkNPS and DeepMet that are already being used to identify novel metabolites or novel drugs with a simple click of a button.

4.7 Prof. Wishart ended by describing how these chemical language models could be used to predict the structures of novel chemical warfare agents and how this information, combined with the tools mentioned earlier, could be used to facilitate the rapid (in seconds) identification of previously unknown or completely novel chemical warfare agents.

4.8 Members of the TWG commented on and discussed a number of themes mentioned by Prof. Wishart, including the need for accurate electrospray ionisation time-of-flight mass spectrometry (EI-TOF-MS) and physico-chemical prediction models, the time constraints connected to traditional methods when compared to ML techniques, and the current constraints of the FraGNNet algorithm. Prof. Wishart further outlined the differences between GC-AutoFit and the Automated Mass Spectral Deconvolution and Identification System (AMDIS), specifically its capability for quantitation and including predicted data, which leads to larger reference database. The TWG members highlighted the need for chemometric tools that can be accessed and used locally and do not rely on Internet-based databases.

5. AGENDA ITEM FIVE – Metabolomics at Repository Scales: Leveraging Mass Spectrometry Big Data to Illuminate Dark Matter

5.1 Prof. Mingxun Wang, from the University of California, Riverside, United States of America, presented the work of his research group on identifying molecules in samples by leveraging mass spectrometry. The group is focusing on MS since this technique provides three principal advantages: high throughput; quantitative analysis; and versatile application. However, as MS—in simple terms—"weighs" the molecules, it cannot differentiate between two chemicals with the same mass but different structures. To overcome this limitation, MS/MS may be used but the identification rate remains low. A single biological sample may contain tens or even hundreds of molecules. Prof. Wang revealed that the identification rate of molecules in a biological sample in 2014 was well below 1%. Today, this rate has grown to 13% and he explained how his work, applying three different strategies, has contributed to this increase.

5.2 In terms of publicly known MS analytes, only 5% to 15% of more than one billion molecules are currently known. To identify these known molecules, comparison with a library of known compounds in a MS/MS library is required. The larger the library, the higher the chances of identifying molecules. To facilitate this process, in 2014

Prof. Wang and his research group decided to crowdsource MS/MS libraries, an idea inspired by other communities such as the Protein Data Bank. As a result, they have developed Global Natural Products Social Molecular Networking (GNPS),[11] a "web-based mass spectrometry ecosystem that aims to be an open-access base for community-wide organization and sharing of raw, processed, or annotated fragmentation mass spectrometry data". Starting at just a few thousand, there are now more than 600,000 spectra in the community library. Prof. Wang noted these have been benchmarked against National Institute of Standards and Technology (NIST) data—the gold standard of spectral libraries—and that their crowdsourced library had equal or better compound identification ratings than commercial libraries, including NIST and MassBank. This strategy increased the overall identification rate from well below 1% to 4%.

5.3 Prof. Wang and his group subsequently adopted their second strategy to expanding knowledge and increasing the identification rate further. This approach focused on considering two structurally similar molecules, differing by a single molecular modification. These structural similarities carry across to the bond strengths and fragmentation patterns, which result in similar tandem mass spectra. Using a tandem mass spectra matching technique, they were able to score two spectra and ascertain whether they are putatively structurally related. However, Prof. Wang noted this technique could only be successfully applied to two molecules differing by a single modification. Fortunately, in the fields of chemistry and biology, multiple modifications are not generally observed in a single step, providing an opportunity to identify single modifications. This approach, known as molecular networking, can be scaled up and applied to all detected molecules in a data set.[12] Prof. Wang highlighted an application where, after identifying a particular molecule in a network and bringing together a network of related molecules, a new molecule could be identified through annotation propagation. This method has been leveraged to discover other new molecules relatively quickly.

5.4 As manual annotation propagation is labour intensive for chemists, Prof. Wang proposed solving the problem computationally and developed a new approach, called ModiFinder, which looks at the peaks that shift and those that do not. If peaks shift, this indicates that the associate substructure must include the modification site and the reverse is true if the peaks do not shift. ModiFinder successfully predicted where a chemical modification occurred in test cases. This work culminated in applying molecular networking on a repository scale—in this case, more than 2,000 public metabolomics data sets containing 60 terabytes of raw data. By infusing the molecular networks together, with 1.1 billion tandem mass spectra, approximately 88,000 putative propagated tandem mass spectra were obtained. Not only did this lead to the current 13% identification rate, but it also yielded a 15% growth in the libraries and a 400% increase in the annotation rate.

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11 Wang, M., J. Carver, V. Phelan, L. Sanchez, N. Garg, Y. Peng, D. Nguyen, et al. "Sharing and Community Curation of Mass Spectrometry Data with Global Natural Products Social Molecular Networking." *Nature Biotechnology* 34, (August 9, 2016): 828–837, https://doi.org/10.1038/nbt.3597.

12 Quinn, R. A., A. V. Melnik, A. Vrbanac, T. Fu, K. A. Patras, M. P. Christy, Z. Bodai, et al. "Global Chemical Effects of the Microbiome Include New Bile-Acid Conjugations." *Nature* 579, no. 7797 (February 26, 2020): 123–29. https://doi.org/10.1038/s41586-020-2047-9.

5.5 Finally, Prof. Wang presented the third strategy they have employed, namely developing a universal computational solution to search for patterns in public data. To this end, they have created a new language—MassQL (Mass Spectrometry Query Language)—to mine repository-scale data.[13] It has been specifically developed to be understandable (for chemists), flexible, scalable, and reusable. He highlighted an example of applying MassQL to organophosphate esters. This identified approximately 338,000 spectra from the 1.1 billion tandem mass spectra publicly available. Unique spectra were then identified and then GNPS was applied to establish the molecular network. A total of 169 molecular families were identified and several new organophosphate esters were discovered as a result.

5.6 The questions posed by the TWG members initially focused on the application of these techniques to identifying products in a chemical reaction matrix, which may be useful from a chemical forensics perspective. Prof. Wang confirmed that MassQL has been used to do this, although it is not always successful since the reaction products need to produce distinctive patterns for it to work. They have also applied reverse metabolomics to make a range of new metabolites and determine whether they have already been seen in public data. This technique could potentially be applied to chemical warfare agents.

5.7 Additional discussion focused on the requirements to access and run GNPS. Prof. Wang explained that GNPS 2.0 is versatile and can be used in three different ways: via a webservices platform; by running workflows on the command line; and by downloading it and running it locally. Furthermore, although the system accesses terabytes of data, a local system does not require a large amount of storage available to run the tools. The level of computational expertise required will depend on the complexity of the task. In some cases, a motivated chemist with experience of Linux will be sufficient: in other cases, when run at scale and with greater computational infrastructure, dedicated expertise will be required. GNPS is also integrated with a mass search tool, known as MASST,[14] which enables a single tandem mass spectrum to be searched against public GNPS spectral libraries and all public tandem MS data sets.

6. AGENDA ITEM SIX – National Measurement Institute – Australian Forensic Drug Laboratory's Profiling Program

6.1 Dr Helen Salouros from the National Measurement Institute (NMI), Australia, opened her presentation with a brief overview of the organisational structure and role of NMI as the Australian Government's national authority on measurement. The Australian Forensic Drug Laboratory is part of the testing and analytical services provided by NMI and is responsible for analysing drugs seized at the border. Over 7,000 samples are analysed annually by the laboratory, with methamphetamine being the drug most frequently analysed in 2024, followed by cocaine and tobacco and related products. Although the volume of novel psychoactive substances analysed, such as synthetic opioids and cannabinoids, is relatively small compared to what is being seen in the United States of America, Dr Salouros noted that a full structural elucidation of these compounds is particularly time-consuming and hampered by the fact there may be no reference materials or spectral data available to assist with interpretation. Samples of

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13 Jarmusch, A. K., A. T. Aron, D. Petras, V. V. Phelan, W. Bittremieux, D. D. Acharya, M. M. Ahmed, et al. "A Universal Language for Finding Mass Spectrometry Data Patterns." August 7, 2022. https://doi.org/10.1101/2022.08.06.503000.

14 For more information, see: https://masst.gnps2.org/.

seized drugs initially undergo chemical analysis, using traditional identification and quantification techniques. If the drug is determined to be cocaine, heroin, or methamphetamine, with a purity of greater than 10%, the sample then undergoes chemical profiling. The laboratory's drug profiling programme dates back to 2001. It initially focused on heroin before being expanded to include cocaine with the aim to determine the geographical origin of the drugs.

6.2 Dr Salouros provided a brief description of heroin production and highlighted the principal sources of the signatures that arise. For example, ultra performance liquid chromatography (UPLC) is used to confirm and quantify the presence of major alkaloids—including morphine, codeine, acetyl codeine, and papaverine—in samples of heroin. The presence and relative quantities of these alkaloids can indicate the geographical region of origin of the heroin. Samples from different countries and regions may be distinguished in this way. Further information can also be provided by GC-MS analysis of by-products in the heroin. Occluded solvents, confirmed using headspace GC-MS, provide information on the particular solvent mixtures used during production, which are also typically region-specific.

6.3 A similar approach may be applied to the analysis of cocaine, where several chemical signatures can be used to determine the origin of the coca leaf and how the cocaine was processed. Again, analysis by GC-MS provides information on alkaloids present, which are dependent on the growing region and the coca leaf species. Headspace GC-MS provides information on specific solvent profiles and enables differentiation of samples. Stable isotope analysis of cocaine using isotope-ration mass spectrometry (IRMS) can provide insights into the growing conditions of the coca plant. The isotopes of nitrogen are influenced by the soil, while those of carbon are affected by the altitude of the growing region. While the geographical origin of the coca leaf can usually be determined, Dr Salouros highlighted recent instances when this was challenging and postulated that this could be a result of storage conditions, extraction from impregnation, or chemical concealment methods which could have affected the cocaine chemical profile.

6.4 Methamphetamine is now the principal drug profiled at the Australian Forensic Drug Laboratory, and in excess of 1,000 samples were processed in 2024 alone. Quantitative NMR spectroscopy is used for purity determination of the methamphetamine; from this analysis any adulterant or diluents can also be identified and quantified. Organic impurity profiling using GC-MS initially provided easy-to-detect chemical profiles, for example samples containing large amounts of route-specific marker compounds. However, in the past 10 to 15 years, the drug landscape has changed such that methamphetamine samples contain little to no organic impurities—almost pharmaceutical grade—thereby providing little information on how these samples have been manufactured. In this case, other signatures can be leveraged, particularly stable isotope ratio analysis, leading to identification of the precursors and pre-precursors used in the manufacture.

6.5 In closing, Dr Salouros emphasised the importance and value of sharing intelligence and set out some key challenges. These included "doing more with less" and how AI and automation can be leveraged in this context, the changing needs of clients, and data mining.

6.6 This presentation elicited a large number of questions. The TWG members were particularly interested in the geolocating work that had been carried out. Dr Salouros stated that work on coca plants had been carried out by the Drug Enforcement Administration in the United States of America and a large number of authentic samples from a range of growing regions had been profiled. This work had been carried out over several decades, with re-evaluation of results. Consequently, a large data set has been generated. Regarding geolocating opium poppies, Dr Salouros explained that while IRMS could potentially be leveraged to provide their geographical origin, it is highly challenging and offers minimal value relative to the effort required.

6.7 Regarding the application of AI in drug profiling, Dr Salouros noted that the use of AI is challenging and that it has only been used in an experimental capacity to date. Dr Salouros noted its potential future application as a quality control measure to verify analysts' work.

7. AGENDA ITEM SEVEN – A Police Perspective on Chemical Forensics and Chemometrics: ENFSI Projects STEFA and ROTOR

7.1 Mr Sami Huhtala, from the National Bureau of Investigation, Finland, provided the Group with an overview of chemical forensics from a police perspective, providing two detailed forensics examples and highlighting two specific projects from the European Network of Forensic Science Institutes (ENFSI). One of his colleagues from the ENFSI projects, Dr Ivo Alberink from the Netherlands Forensic Institute, joined the meeting virtually to help answer any statistics-related questions. Mr Huhtala opened his presentation with an introduction to the work of the Forensic Laboratory, which is part of the National Bureau of Investigation and the sole police forensics laboratory in Finland.

7.2 Mr Huhtala described two cases in which chemical forensics methods played a critical role. The first related to identifying the source of an oil spill in the environment. He underscored the importance of selecting multiple sampling locations and the availability of detailed sampling guidelines for the police and coastguard officials. He discussed the changing nature of the spill, and consequently the chemical profile, due to weathering processes such as evaporation, biodegradation, oxidation, and photolysis, and the challenges this presents. The Forensic Laboratory has reference samples for the comparison and identification of different oils and research has been performed on weathering processes and the impact on the chemical profiles examined. Mr Huhtala noted that algorithms have been developed to account for weathering and to compensate for its effects on the results. In order to compare oil samples and assess the degree of similarity, the Forensic Laboratory has developed a series of likelihood ratios, which are derived through a statistical model. Likelihood ratios provide an evaluation of the strength of evidence by comparing two competing hypotheses and ensure a consistent and transparent approach. This approach is particularly useful in cases in which there is significant expert knowledge but limited database resources available. A conclusion scale has also been developed, converting the likelihood ratio to a value between minus six and plus six, to provide a more easily communicable level of confidence in the conclusions reached.

7.3 The second forensics example focused on cocaine. Mr Huhtala highlighted that wastewater studies have shown that cocaine use since 2013 has continued to rise in Finland. He provided an overview of the production of cocaine from coca leaves and noted that the chemical profiling of cocaine is based on the analysis of different compounds found in the cocaine product, including alkaloids from the leaves, impurities, occluded solvents, adulterants, and diluents. He further noted the growing trend of producing so-called "black cocaine", a method used by drug traffickers to evade detection. This process involves mixing cocaine with other substances (such as charcoal or dyes) to create a black or dark-coloured solid, disguising it and making it undetectable by conventional drug tests. This can significantly increase the number of additional chemicals present in a sample, affecting the chemical profile. Furthermore, bulk cocaine may consist of multiple batches (of coca paste, for example)—a result of the current approach of subcontracting different stages in the production process—which can lead to a new chemical profile. Consequently, having the "same origin" only applies to the point in the production process at which these batches were combined, which currently remains challenging to determine. Cocaine produced from the same mix of coca paste can lead to different chemical profiles, arising from slight differences in the processing method. The high purity of cocaine nowadays means that the levels of alkaloids other than cocaine are very low (trace level), and occluded solvents are now the best source of information for the Forensic Laboratory.

7.4 Mr Huhtala provided an overview of how chemical profiling is undertaken at the Forensic Laboratory, highlighting key investigative questions addressed and summarising the analytical methods. He also discussed some of the limitations associated with chemical profiling, such as the number of samples received, the type of data that can be obtained from the samples, and the nature of the forensic question. He underscored the importance of having an up-to-date database of samples that represents the current drug landscape.

7.5 Two ENFSI chemometrics projects were then presented.[15,16,17] The first, Steps Towards a European Forensic Science Area (STEFA), was a three-year project which aimed to provide chemists with easier access to existing chemometric methods. The outputs included the ENFSI guideline booklet,[18] which compiles common chemometrics practices, and a software tool, ChemoRe,[19] which provides easy and intuitive access to the powerful functions of the statistical programming language R. Following on from STEFA is the ongoing ROTOR project, which will provide guidance to forensic chemists on method selection and will deliver an update to ChemoRe. Mr Huhtala described ChemoRe, noting that it has a web-based interface and can be downloaded at no cost, and then provided a demonstration.

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15 Bovens, M., B. Ahrens, I. Alberink, A. Nordgaard, T. Salonen, and S. Huhtala. "Chemometrics in Forensic Chemistry — Part I: Implications to the Forensic Workflow." *Forensic Science International* 301 (August 2019): 82–90. https://doi.org/10.1016/j.forsciint.2019.05.030.

16 Salonen, T., B. Ahrens, M. Bovens, J. Eliaerts, S. Huhtala, A. Nordgaard, and I. Alberink. "Chemometrics in Forensic Chemistry — Part II: Standardized Applications – Three Examples Involving Illicit Drugs." *Forensic Science International* 307 (February 2020): 110138. https://doi.org/10.1016/j.forsciint.2019.110138.

17 Huhtala, S., A. Nordgaard, B. Ahrens, I. Alberink, T. Korpinsalo, and M. Bovens. "Chemometrics in Forensic Chemistry – Part III: Quality Assessment and Interpretation of Chemometric Output." *Forensic Science International* 348 (July 2023): 111612. https://doi.org/10.1016/j.forsciint.2023.111612.

18 See: https://enfsi.eu/wp-content/uploads/2021/09/Guideline-for-the-use-of-Chemometrics-in-Forensic-Chemistry.pdf.

19 ChemoRe is available for download from the ENFSI website: https://enfsi.eu/downloads/.

7.6 Following the presentation, the TWG members asked about the likelihood ratios, including whether there is a common approach on how to calculate them or a common system applied to multiple laboratories, and whether workflows are available in the ENFSI guidelines. There were questions regarding the effects of subcontracting stages of cocaine production on the chemical profiles and batch effects—and consequent differences in chemical profile—observed in methamphetamine production. The discussion concluded with a focus on multivariate data analysis, including the quantity of training data required to generate significant likelihood ratios, unit variance scaling, and benchmarking.

8. AGENDA ITEM EIGHT – Evidence-based assurance and verification of Australian agriculture provenance

8.1 Dr Nina Welti, from the Commonwealth Scientific and Industrial Research Organisation (CSIRO), Australia, provided an overview of her organisation's research into agricultural verification, underscoring the increasing demand for transparent, evidence-based food provenance systems. While regulatory frameworks play a role, she highlighted the growing interest among consumers, producers, and authorities in ensuring supply chain transparency, food safety, environmental responsibility, and authenticity. She emphasised that customers paying premiums for verified claims require objective evidence, reinforcing the need for trusted tools to assure food origins.

8.2 Traditional techniques such as stable isotope analysis and elemental composition face limitations due to siloed data sources and the need for extensive reference data sets. She highlighted that these limitations could be overcome by using landscape and mechanistic models in combination with AI-driven analytics, and that, consequently, stable isotope signatures could be used to enhance agricultural provenance verification. She acknowledged spatial limitations, noting that current models typically differentiate sample locations only when they are 100 to 250 km apart.

8.3 Dr Welti presented case studies demonstrating the forensic application of isotope analysis, including its role in verifying illegally harvested sandalwood,[20] where stable isotope ratios (carbon, oxygen, and strontium) helped confirm that confiscated samples did not originate from their declared source. In another example, cherries were classified using a combination of isotope analysis and near-infrared spectroscopy on both fruit and soil, improving geographical accuracy. Dr Welti also discussed the application of isotope analysis in verifying sustainability claims in textiles, particularly in efforts to reduce methane emissions in sheep farming.

8.4 Dr Welti explained the approach used by CSIRO to predict the geographical origin of agricultural products by integrating landscape modelling, isotopic data, and machine learning techniques.[21] By leveraging soil geochemical signatures, groundwater isotopes, and environmental variables, probabilistic models that estimate the likelihood of a product originating from a specific region can be generated. She noted that this

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20 Bunney, E., F. A. McInerney, E. Dormontt, A. Malik, N. Welti, D. Wilkins, M. Plant, et al. "Safeguarding Sandalwood: A Review of Current and Emerging Tools to Support Sustainable and Legal Forestry." *Plants, People, Planet* 5, no. 2 (December 18, 2022): 190–202. https://doi.org/10.1002/ppp3.10349.

21 Coggins, S., B. P. Malone, U. Stockmann, M. Possell, and A. B. McBratney. "Towards Meaningful Geographical Indications: Validating Terroirs on a 200 km^2 Scale in Australia's Lower Hunter Valley." *Geoderma Regional* 16 (March 2019). https://doi.org/10.1016/j.geodrs.2019.e00209.

method refines existing provenance tools by combining point-based data sets with AI-driven spatial interpolation, effectively subdividing Australia into chemically distinct geographical regions. While this combinatorial approach is not new, it is efficient and effective, and incorporating AI methods can create dynamic models as data coverage increases. Dr Welti highlighted that the creation of a multi-elemental signature improves the probability and uniqueness for a given location.

8.5 Dr Welti discussed the role of isotope models in refining provenance verification, especially their use in linking environmental attributes to agricultural products.[22] She explained that stable isotope ratios of elements like oxygen, hydrogen, and strontium vary geographically due to environmental factors such as precipitation, soil composition, and plant uptake. By integrating spatially interpolated isoscapes with machine learning, multi-elemental signatures that improve the accuracy of geographical origin predictions can be generated. However, she noted that while these models provide valuable insights, they must account for biological transformations—for example, how plants alter isotope compositions through evapotranspiration. She underscored how efficient data harmonisation is crucial.

8.6 A major challenge in food provenance research, Dr Welti stressed, is data accessibility. While extensive environmental stable isotope data sets exist, they remain fragmented across various locations, in differing formats. To address this, CSIRO is collaborating with key Australian Government organisations to create a national data asset for stable isotopes. This initiative aims to harmonise data sets, improve interoperability, and support broader research applications. A platform has been developed that connects to data sets in a variety of formats, translating them into, and reporting out with, common ontologies, thereby enabling disparate data to be harmonised.[23] Dr Welti further emphasised the importance of privacy-preserving data-sharing frameworks. She described innovative approaches, such as synthetic data augmentation, which enable secure information sharing without compromising commercial sensitivities.

8.7 In concluding, Dr Welti emphasised that predictive modelling and AI-driven analytics will be critical to the future of food provenance, and highlighted a data fusion method for hyperspectral measurements for elemental composition in mixed matrices. However, for scientific advancements to be widely adopted, she stressed the importance of developing practical, rapid assessment tools that producers can integrate into supply chain operations.

8.8 Following this presentation, members of the TWG raised a number of questions relating to existing platforms and approaches used as a source of inspiration, data privacy (including consideration of data protection versus data anonymisation), and the universal applicability of the methods employed, given they have been developed in a geographically isolated and unique environment.

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22 Munroe, S. E., G. R. Guerin, F. A. McInerney, I. Martín-Forés, N. Welti, M. Farrell, R. Atkins, and B. Sparrow. “A Vegetation Carbon Isoscape for Australia Built by Combining Continental-Scale Field Surveys with Remote Sensing.” *Landscape Ecology* 37, no. 8 (July 5, 2022): 1987–2006. https://doi.org/10.1007/s10980-022-01476-y.

23 For more information, see: https://app.isotopes.au/#/.

9. AGENDA ITEM NINE – Subgroups breakout sessions

See agenda item two.

10. AGENDA ITEM TEN – Casework examples of fire debris analysis and miscellaneous chemical investigations in the Netherlands

10.1 In his two-part presentation, Dr Michiel Grutters, from the Netherlands Forensic Institute, briefly discussed the Institute's work in traditional chemical forensic disciplines, such as illicit drugs, fire debris analysis, toxicology, and environmental investigations. He also highlighted that many questions posed by the police during investigations do not fit into these traditional categories, instead falling under the broader category of miscellaneous chemical investigations.

10.2 Following this scene setting, Dr Grutters provided a brief introduction to fire debris analysis, which aims to determine whether fire debris samples—pieces of evidence—contain ignitable liquids, such as gasoline, denatured spirits, white spirit, and/or lamp oil, among others. At the scene of a fire, the police use arson dogs to detect and locate areas where ignitable liquids may be present and suitable samples can be taken. Due to the volatile nature of the ignitable liquids, Dr Grutters stressed the importance of packaging these samples, which include wood and carpet, in either a glass jar or a fire debris bag to preserve the evidence. This volatility is then exploited during the analysis process where the vapour from the sample may be directly sampled (direct headspace) or is concentrated on activated charcoal, solid phase microextraction (SPME) fibres, or Tenax tubes (preferred). Analysis is subsequently conducted using GC-MS. The volatile constituents are identified and their spectral patterns interpreted. A number of effects may distort the observed patterns of the volatiles and complicate interpretation. These effects include evaporation, microbial degradation, and volatile components from the burned matrix (such as polypropylene and high-density polyethylene).

10.3 Dr Grutters then presented a specific case example where a gasoline comparison was requested, with gasoline from a fire scene compared with residue in a plastic bottle from a suspect's house. In order to determine the evidential strength of the comparison results, two opposing hypotheses were constructed and a likelihood ratio subsequently determined. To explore the hundreds of different components in gasoline, a Likens-Nickerson simultaneous distillation-extraction was performed. Consequently, several features of the gasoline composition could be distinguished, including oxygenates, alkylate components,[24] dicyclopentadienes, and the gasoline fingerprint.

10.4 Using the likelihood ratio approach, a statistical model is applied and a score—a measure of similarity—calculated.[25] A final likelihood ratio is calculated from the individual likelihood ratios of the aliphatic and aromatic components. This final likelihood ratio assists in the final expert opinion. Dr Grutters noted that the statistical model used had been trained with data from both a local and a national gasoline

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24 Peschier, Leo J.C., Michiel M.P. Grutters, and Jeanet N. Hendrikse. "Using Alkylate Components for Classifying Gasoline in Fire Debris Samples." *Journal of Forensic Sciences* 63, no. 2 (May 30, 2017): 420–30. https://doi.org/10.1111/1556-4029.13563.

25 Vergeer, P., J.N. Hendrikse, M.M.P. Grutters, and L.J.C. Peschier. "A Method for Forensic Gasoline Comparison in Fire Debris Samples: A Numerical Likelihood Ratio System." *Science & Justice* 60, no. 5 (September 2020): 438–50. https://doi.org/10.1016/j.scijus.2020.06.002.

database, containing more than 2,000 samples of gasoline from gas stations throughout the Netherlands. The model was validated using an independent data set consisting of 104 weathered gasoline samples spiked (partially evaporated) on a variety of matrices.

10.5 The second case example presented by Dr Grutters related to a miscellaneous chemical investigation to compare a brown substance found on the shoe of a suspect with a sample of barbecue sauce at the scene of a burglary. Broad screening was performed using a combination of techniques and as many compounds as possible were elucidated. This analysis approach provided a lot of data and data processing software was leveraged.

10.6 Dr Grutters underscored the importance of hypothesis formulation, particularly alternating hypotheses, as this has a significant effect on the likelihood ratio and the weight of the evidence. He further noted that, ideally, hypotheses should be formulated in conjunction with the investigating judge.

10.7 Following the presentation, the members of the TWG further discussed ignitable liquids. They noted that turpentine is a complex mixture of terpenes, which are also naturally present in wood, particularly in softwood species like pine and spruce. This overlap makes it challenging to distinguish between turpentine and wood-derived terpenes. The Group also considered batch-to-batch variations in gasoline. Despite these variations, Dr Grutters stated that samples originating from the same source can typically be identified.

10.8 To monitor instrument performance, a gasoline quality control sample is always measured. Furthermore, Dr Grutters emphasised that gas chromatography-flame ionisation detection (GC-FID) analysis is a very robust technique and used extensively, with the statistical model based on data from this instrument. However, despite the model's utility, it has limitations and is not relied upon completely—any unexpected results are manually reviewed.

10.9 The TWG members noted with interest the broad screening approach adopted in the second case example but agreed that further work must be undertaken in order for this to be analytically acceptable. Lastly, discussion focused on the formulation of alternating hypotheses, the importance of agreeing them with the investigating judge to ensure the most suitable one is used, and their utility in cases with small data sets.

11. AGENDA ITEM ELEVEN – Challenges for chemical forensics and chlorine profiling in concrete

11.1 Dr Mirjam de Bruin-Hoegée, from the Organisation for Applied Scientific Research (TNO), the Netherlands, opened her presentation by describing the relevance of chemical forensics within the context of the Chemical Weapons Convention, highlighting methods commonly used in profiling nerve agents. Dr de Bruin-Hoegée noted the key challenges relating to the various stages of forensic investigations. For example, during sample collection, these challenges included difficulty in sensitively detecting chemical attribution signatures at trace levels using portable techniques and

rapid degradation in the environment.[26] During laboratory analysis, detection may be hampered by matrix interference or identification of possible unknown toxic chemicals may be difficult. She emphasised the need for research to represent real-world cases, highlighting concentration limits in particular, and the important role interlaboratory comparisons and data sharing can play in developing robust and reproducible analytical methods.[27] Regarding forensic reporting and legal accountability, Dr de Bruin-Hoegée described the application of data science in this space. She noted that while AI can enhance the speed and efficiency of chemical attribution analyses, the lack of large data sets and explainable models remains a barrier to progress. In concluding the first part of her presentation, Dr de Bruin-Hoegée noted that new types of evidence and analytical profiling strategies can support forensic investigations and that data science can play a key role in innovating forensic attribution research.

11.2 In the second part of her presentation, Dr de Bruin-Hoegée focused on identifying selective markers for chlorine gas exposure in concrete. She explained that verifying chlorine exposure is difficult due to its high reactivity, rapid evaporation, and formation of non-specific markers. While most research to date has centred on biomedical samples,[28] TNO has also investigated plant-based markers for chlorine exposure.[29,30] However, collecting biomedical samples may pose safety and ethical challenges and plant availability may be limited in urban environments. In contrast, concrete—the world's most abundant building material—offers a more accessible and practical alternative for sampling, helping to overcome these challenges.

11.3 Dr de Bruin-Hoegée outlined the research goal: to identify selective markers of chlorine gas exposure in concrete using mass spectrometric techniques combined with machine learning methods. Using traditional chemical forensics techniques, it was envisaged that the research would confirm exposure to chlorine gas and distinguish it from other chlorine-generating materials. Samples of two types of hardened concrete and two types of cement were each exposed to sodium hypochlorite, pool bleach, household bleach, and chlorine gas. A total of 280 experiments were carried out, including non-exposed and negative samples. During analysis, untargeted screening and targeted analysis were performed, followed by data processing and data analysis. Analysis by GC-MS identified 32 chlorinated markers, whereas analysis by liquid chromatography-high resolution tandem mass spectrometry (LC-HRMS/MS) identified in excess of 4,500 chlorinated

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26 Kranenburg, R. F., H.-J. Ramaker, S. Sap, and A. C. van Asten. "A Calibration Friendly Approach to Identify Drugs of Abuse Mixtures with a Portable Near-infrared Analyzer." *Drug Testing and Analysis* 14, no. 6 (February 9, 2022): 1089–1101. https://doi.org/10.1002/dta.3231.

27 Holmgren, K. Höjer, H. Hakulinen, R. Norlin, M. de Bruin-Hoegée, M. Spiandore, S. Qi See, R. Webster, et al. "Interlaboratory Comparison Study of a Chemical Profiling Method for Methylphosphonic Dichloride, a Nerve Agent Precursor." *Forensic Chemistry* 33 (May 2023): 100473. https://doi.org/10.1016/j.forc.2023.100473.

28 Bruin-Hoegée, M. de, I. M. van Damme, T. van Groningen, D. van der Riet-van Oeveren, D. Noort, and A. C. van Asten. "Elucidation of in Vitro Chlorinated Tyrosine Adducts in Blood Plasma as Selective Biomarkers of Chlorine Exposure." *Chemical Research in Toxicology* 35, no. 6 (May 27, 2022): 1070–79. https://doi.org/10.1021/acs.chemrestox.2c00053.

29 Bruin-Hoegée, M. de, L. Lamriti, J. P. Langenberg, R. C. Olivier, L. Fun Chau, M. J. van der Schans, D. Noort, and A. C. van Asten. "Verification of Exposure to Chemical Warfare Agents through Analysis of Persistent Biomarkers in Plants." *Analytical Methods* 15, no. 2 (2023): 142–53. https://doi.org/10.1039/d2ay01650h.

30 Bruin-Hoegée, M. de, M. J. van der Schans, J. P. Langenberg, and A. C. van Asten. "Biomarker Profiling in Plants to Distinguish between Exposure to Chlorine Gas and Bleach Using LC-HRMS/MS and Chemometrics." *Forensic Science International* 358 (May 2024): 112022. https://doi.org/10.1016/j.forsciint.2024.112022.

markers. Verification with reference standards confirmed five markers with GC-MS and one marker with liquid chromatography-tandem mass spectrometry (LC-MS/MS) that may be specific to chlorine exposure. In conclusion, Dr de Bruin-Hoegée noted that distinguishing markers for chlorine and bleach exposure were identified and that chemometrics may facilitate the selection of promising markers. She recalled that for unambiguous verification, synthetic reference standards are required, and highlighted that well-validated likelihood ratio models could facilitate forensic classifications.

11.4 Following the presentation, members of the TWG posed questions on the different types of concrete investigated, other potential building materials suitable for chlorine profiling, and sampling methods, especially from an operational perspective. They discussed the possible effects of chlorinated solvents such as dichloromethane used in the extraction process, the analytical techniques selected, and the effect environmental factors might have on the chemical profile of samples. Lastly, it was suggested that demonstrating that bleach was not used through hypothesis formulation may be easier than proving that chlorine gas was used.

12. AGENDA ITEM TWELVE – Subgroups breakout sessions

See agenda item two.

13. AGENDA ITEM THIRTEEN – Group discussion

See agenda item two.

14. AGENDA ITEM FOURTEEN – Closing remarks and any other business

Dr Bossée thanked the TWG members for their contributions and discussions during both the intersessional period and the meeting itself. Dr Ovenden noted that the draft report would be available on Microsoft Teams once some final additions had been made, and encouraged all subgroup members to review and edit the text. He thanked the external speakers, in addition to the OPCW for providing organisational and logistical assistance. No additional points were raised.

15. AGENDA ITEM FIFTEEN – Closure of the meeting

The Chairperson ended the meeting at 16:53 (CET) on 24 January 2025.

ACKNOWLEDGEMENTS

The TWG members thank the guests and members of the Secretariat who participated in discussions. The TWG also wishes to acknowledge Ms Ernesa Ademagić of the OPCW Office of Strategy and Policy for her support and contributions to the meeting and its preparations. Lastly, the TWG thanks the OPCW Director-General for his establishment and support of the TWG, and acknowledges the generous contributions of the European Union and the United States of America that help to cover the costs of the Group's work.

Annex: List of Participants at the Fourth Meeting of the Scientific Advisory Board's Temporary Working Group on Chemical Forensics

Annex

LIST OF PARTICIPANTS AT THE FOURTH MEETING OF THE SCIENTIFIC ADVISORY BOARD'S TEMPORARY WORKING GROUP ON CHEMICAL FORENSICS

	Participant	**Institution**
1.	Prof. Arian van Asten	University of Amsterdam, Netherlands
2.	Dr Crister Åstot*	Swedish Defence Research Agency (FOI), Sweden
3.	Capt. Elma Biscotti*	Scientific and Technical Research Institute for Defense (retired), Argentina
4.	Dr Anne Bossée* (Chairperson of the TWG)	DGA CBRN Defence, France
5.	Dr Grégoire Delaporte	DGA CBRN Defence, France
6.	Ms Anne-Marie Fortin	United Nations Office on Drugs and Crime, International
7.	Dr Hanna Hakulinen	Finnish Institute for Verification of the Chemical Weapons Convention (VERIFIN), Finland
8.	Ms Ang Lee Hwi	DSO National Laboratories, Singapore
9.	Prof. Imee Su Martinez*	University of the Philippines Diliman, Philippines
10.	Dr Simon Ovenden (Vice-Chairperson of the TWG)	Defence Science and Technology Group, Australia
11.	Dr Meehir Palit*	Defence Research and Development Organisation, India
12.	Mr Günter Povoden	CBRN Defence Centre, Austrian Armed Forces, Austria
13.	Prof. Ines Primožič*	University of Zagreb, Croatia
14.	Dr Sarah Stubbs	Defence Science and Technology Laboratory, United Kingdom of Great Britain and Northern Ireland
15.	Dr Hongmei Wang	State Key Laboratory of NBC Protection for Civilian, China
16.	Dr Audrey Williams	Lawrence Livermore National Laboratory, United States of America
	Invited Speakers	**Institution**
17.	Dr Ivo Alberink	Netherlands Forensic Institute, Netherlands
18.	Dr Mirjam de Bruin-Hoegée	TNO, Netherlands
19.	Dr Georgios Gkatzelis	Forschungszentrum Jülich GmbH, Germany
20.	Dr Michiel Grutters	Netherlands Forensic Institute, Netherlands
21.	Mr Sami Huhtala	National Bureau of Investigation, Finland
22.	Dr Helen Salouros	National Measurement Institute, Australia
23.	Prof. Mingxun Wang	University of California, Riverside, United States of America
24.	Dr Nina Welti	CSIRO, Australia
25.	Prof. David Wishart	University of Alberta, Canada
	Technical Secretariat Staff	**Division**
26.	Dr Peter Hotchkiss (Secretary to the SAB)	Office of Strategy and Policy

* Member of the SAB.

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